Abstract Submitted
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Bound and Unbound: Stabilizing the Anionic States of Adamantane through Functionalization[1] ZACHARY POZUN, VAMSEE VOORA, University of Pittsburgh, MICHAEL FALCETTA, Grove City College, KENNETH JORDAN, University of Pittsburgh — Adamantane is the simplest diamondoid, which are nanostructures of carbon with a diamond-like cage structure. Although diamondoids have been reported to have negative electron affinities (EA),[2] calculating an EA for an unbound anion is not straightforward because the localized anion state is strongly coupled to the continuum. In order to determine the energy and lifetime of temporary anions, we apply the stabilization method, where the exponents of the diffuse basis functions centered on the carbon atoms are scaled during equation-of-motion calculations; the energies of the anionic states are relatively insensitive to the scaling factor as compared to the continuum states.[3] We use this method in order to identify temporary anion states and their associated energies and lifetimes. We also demonstrate that these states can be tuned in energy based substituting the adamantane cage with substituents that either withdraw or donate charge into the carbon-carbon backbone. Thus, the unique optoelectric properties of small diamondoids can be properly calculated and easily tuned.

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[2]N. D. Drummond, A. J. Williamson, R. J. Needs, and G. Galli. Phys. Rev. Lett., 95, 096801 (2005).
[3]J. S.-Y. Chao, M. F. Falcetta, and K. D. Jordan. J. Chem. Phys., 93(2), 1125-1134 (1990)

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